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* * * * * Welcome to STN International * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2	Jan 25	BLAST(R) searching in REGISTRY available in STN on the Web
NEWS 3	Jan 29	FSTA has been reloaded and moves to weekly updates
NEWS 4	Feb 01	DKILIT now produced by FIZ Karlsruhe and has a new update frequency
NEWS 5	Feb 19	Access via Tymnet and SprintNet Eliminated Effective 3/31/02
NEWS 6	Mar 08	Gene Names now available in BIOSIS
NEWS 7	Mar 22	TOXLIT no longer available
NEWS 8	Mar 22	TRCTHERMO no longer available
NEWS 9	Mar 28	US Provisional Priorities searched with P in CA/CAPLUS and USPATFULL
NEWS 10	Mar 28	LIPINSKI/CALC added for property searching in REGISTRY
NEWS 11	Apr 02	PAPERCHEM no longer available on STN. Use PAPERCHEM2 instead.
NEWS 12	Apr 08	"Ask CAS" for self-help around the clock
NEWS 13	Apr 09	BEILSTEIN: Reload and Implementation of a New Subject Area
NEWS 14	Apr 09	ZDB will be removed from STN
NEWS 15	Apr 19	US Patent Applications available in IFICDB, IFIPAT, and IFIUDB
NEWS 16	Apr 22	Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS
NEWS 17	Apr 22	BIOSIS Gene Names now available in TOXCENTER
NEWS 18	Apr 22	Federal Research in Progress (FEDRIP) now available
NEWS 19	Jun 03	New e-mail delivery for search results now available
NEWS 20	Jun 10	MEDLINE Reload
NEWS 21	Jun 10	PCTFULL has been reloaded
NEWS EXPRESS		February 1 CURRENT WINDOWS VERSION IS V6.0d, CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP), AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002
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NEWS INTER		General Internet Information
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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 08:42:09 ON 20 JUN 2002

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

	ENTRY	SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 08:42:23 ON 20 JUN 2002
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STRUCTURE FILE UPDATES: 18 JUN 2002 HIGHEST RN 431976-32-8
DICTIONARY FILE UPDATES: 18 JUN 2002 HIGHEST RN 431976-32-8

TSCA INFORMATION NOW CURRENT THROUGH January 7, 2002

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES
for more information. See STNote 27, Searching Properties in the CAS
Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>

Uploading lauren1.str

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 08:42:41 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 35 TO ITERATE

100.0% PROCESSED	35 ITERATIONS	16 ANSWERS
SEARCH TIME: 00.00.01		

FULL FILE PROJECTIONS:	ONLINE	**COMPLETE**
	BATCH	**COMPLETE**
PROJECTED ITERATIONS:	346 TO	1054
PROJECTED ANSWERS:	80 TO	560

L2 16 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 08:42:46 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 755 TO ITERATE

100.0% PROCESSED	755 ITERATIONS	334 ANSWERS
SEARCH TIME: 00.00.02		

L3 334 SEA SSS FUL L1

=>

Uploading lauren2.str

L4 STRUCTURE UPLOADED

=> ed

ED IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> d

L4 HAS NO ANSWERS

L4 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l4

SAMPLE SEARCH INITIATED 08:43:35 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 35 TO ITERATE

100.0% PROCESSED 35 ITERATIONS

0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 346 TO 1054

PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L4

=> s l4 full

FULL SEARCH INITIATED 08:43:41 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 755 TO ITERATE

100.0% PROCESSED 755 ITERATIONS

6 ANSWERS

SEARCH TIME: 00.00.01

L6 6 SEA SSS FUL L4

=> fil .search

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

281.70

281.91

FILE 'MEDLINE' ENTERED AT 08:45:38 ON 20 JUN 2002

FILE 'CAPLUS' ENTERED AT 08:45:38 ON 20 JUN 2002

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FILE 'BIOSIS' ENTERED AT 08:45:38 ON 20 JUN 2002

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FILE 'USPATFULL' ENTERED AT 08:45:38 ON 20 JUN 2002

CA INDEXING COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'EMBASE' ENTERED AT 08:45:38 ON 20 JUN 2002

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=> d his

(FILE 'HOME' ENTERED AT 08:42:09 ON 20 JUN 2002)

FILE 'REGISTRY' ENTERED AT 08:42:23 ON 20 JUN 2002

L1 STRUCTURE UPLOADED
L2 16 S L1
L3 334 S L1 FULL
L4 STRUCTURE UPLOADED
L5 0 S L4
L6 6 S L4 FULL

FILE 'MEDLINE, CAPLUS, BIOSIS, USPATFULL, EMBASE' ENTERED AT 08:45:38 ON
20 JUN 2002

=> s l6

L7 7 L6

=> dup rem l7

PROCESSING COMPLETED FOR L7

L8 7 DUP REM L7 (0 DUPLICATES REMOVED)

=> d ibib ab hitstr 1-

YOU HAVE REQUESTED DATA FROM 7 ANSWERS - CONTINUE? Y/(N):y

L8 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2000:227727 CAPLUS
 DOCUMENT NUMBER: 132:271477
 TITLE: Divalent lanthanide metal complexes
 INVENTOR(S): Christou, Victor; Salata, Oleg Victorovich; Shipley, Christopher
 PATENT ASSIGNEE(S): Isis Innovation Limited, UK
 SOURCE: PCT Int. Appl., 36 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000018851	A1	20000406	WO 1999-GB3201	19990924
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MM, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZM, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9961053	A1	20000417	AU 1999-61053	19990924
EP 1115808	A1	20010718	EP 1999-947674	19990924
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				

PRIORITY APPLN. INFO.: GB 1998-20805 A 19980925
 WO 1999-GB3201 W 19990924

AB Light-emitting devices are described which employ complexes contg. a lanthanide (esp. Eu, Sm or Yb) cation complexed with 1 to 3 polydentate ligands. The polydentate ligands preferably contain .gtoreq.1 1H-pyrazol-1-yl groups, such as tris(1H-pyrazol-1-yl)borate anions. Selected complexes are claimed, as are methods for prepg. them by

reacting the divalent cation with the complex ions in soln. and then sepg. the product from the soln.

IT 157409-94-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (divalent lanthanide metal complexes with polydentate ligands and their prepn. and electroluminescent devices using them)

RN 157409-94-4 CAPLUS

CN Borate(1-), tris(4,5-dihydro-1H-benz[g]indazolato-.kappa.N2)hydro-, potassium, (T-4)- (9CI) (CA INDEX NAME)

L8 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1998:805731 CAPLUS
 DOCUMENT NUMBER: 130:73617
 TITLE: Organometallic complexes
 INVENTOR(S): Christou, Victor
 PATENT ASSIGNEE(S): Isis Innovation Ltd., UK
 SOURCE: PCT Int. Appl., 38 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9855561	A1	19981210	WO 1998-GB1587	19980601
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MM, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9876681	A1	19981221	AU 1998-76681	19980601
EP 988353	A1	20000329	EP 1998-924488	19980601
R: BE, DE, ES, FR, GB, IT, NL				
JP 2002513440	T2	20020508	JP 1999-501831	19980601

PRIORITY APPLN. INFO.: GB 1997-11237 A 19970602
 WO 1998-GB1587 W 19980601

OTHER SOURCE(S): MARPAT 130:73617

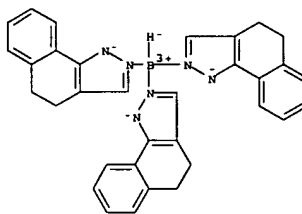
AB Light-emitting devices are described which employ organometallic complexes comprising a lanthanide metal cation complexed with 1-3 polydentate ligands contg. .gtoreq.1 (un)substituted pyrazolyl groups optionally fused with (un)substituted heterocyclic or carbocyclic (non)arom. ring systems, with a coordinate bond formed between the metal and one of the nitrogen atoms of the pyrazolyl rings. Preferably, the ligands comprise trispyrazolyl borate derivs. Organometallic compds. suitable for the devices are also claimed, as are methods of producing them entailing the reaction of the ligands with a cation followed by sepn. of the products. Compns. combining the compds. with a matrix material are also described. Use in electroluminescent flat panel displays is also described.

IT 157409-94-4 217956-54-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (lanthanide-pyrazolyl deriv. complexes and electroluminescent devices and displays using them)

RN 157409-94-4 CAPLUS

CN Borate(1-), tris(4,5-dihydro-1H-benz[g]indazolato-.kappa.N2)hydro-, potassium, (T-4)- (9CI) (CA INDEX NAME)

L8 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)

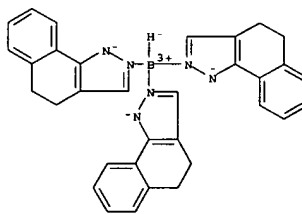


● K⁺

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

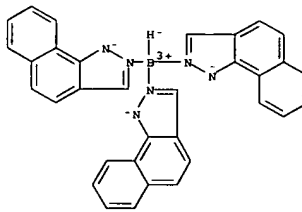
FORMAT

L8 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



● K⁺

RN 217956-54-2 CAPLUS
 CN Borate(1-), tris(1H-benz[g]indazolato-.kappa.N2)hydro-, potassium, (T-4)- (9CI) (CA INDEX NAME)



● K⁺

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

LB ANSWER 3 OF 7 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1997:643548 CAPLUS

DOCUMENT NUMBER: 127:302404

TITLE: Hydrotris(indazolyl)borates: Homoscorpionates with Tunable Regiochemistry

AUTHOR(S): Rheingold, Arnold L.; Haggerty, Brian S.; Yep, Glenn P. A.; Trofimenko, Swiatoslaw

CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Delaware, Newark, DE, 19716, USA

SOURCE: Inorganic Chemistry (1997), 36(22), 5097-5103

CODEN: INOCAJ; ISSN: 0020-1669

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Hydrotris(indazolyl)borates contg. diverse substituents on the indazole ring and representing two types of regiochemistries were synthesized. Indazoles with a 7-alkyl substituent or a 6,7-fused benzo ring formed ligands with B bonded to the less hindered N-2 (=Tp3Bo), while those with alkyl or aryl substituents in any other position yielded ligands with B bonded to the more hindered N-1 (=Tp4Bo), thus being the 1st example of homoscorpionates with 4,5-substituents. Octahedral homo- and

heteroleptic complexes of Co, Fe, and Zn were prepd. and characterized, as well as complexes [M(L)(NCS)], [Mo(L)(CO)2(.eta.3-CH2CMeCH2)], [Rh(L)(COD)], and [Rh(L)(CO)2]. X-ray crystallog. provided structures of [Rh(HB(3-methylindazol-1-yl)3)(COD)] (space group P21/n; a 11.766(2), b 16.189(2), c 15.149(2) .ANG.; .beta. 92.51(1).degree.; Z = 4; R = 0.0306 for 4318 independent reflections), [Co(HB(7-methylindazol-2-yl)3)(HB(3-neopentylpyrazol-1-yl)3)] (space group P.hivin.1; a 13.368(4), b 13.652(4), c 16.203(9) .ANG.; .alpha. 73.73(4), .beta. 71.26(3), .gamma. 63.54(2).degree.; Z = 2; R = 0.0761 for 7721 independent reflections), and

[Co(hydrotris(3-methyl-2H-benz[g]indazol-2-yl)borate)(hydrotris(3-neopentylpyrazol-1-yl)borate)].cntdot.C6H5CN (space group P.hivin.1; a 13.216(6), b 13.706(4), c 17.881(6) .ANG.; .alpha. 73.79(2), .beta. 86.71(3), .gamma. 85.61(3).degree.; Z = 2; R = 0.1138 for 6698 independent reflections).

IT 158989-18-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

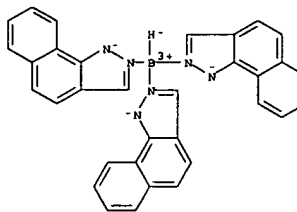
(for prepn. of transition metal indazolylborate complexes)

RN 158989-18-5 CAPLUS

CN Borate(1-), tris(1H-benz[g]indazolato-.kappa.N2)hydro-, thallium(1+), (T-4)- (9CI) (CA INDEX NAME)

LB ANSWER 3 OF 7 CAPLUS COPYRIGHT 2002 ACS

(Continued)



● Tl(I) +

LB ANSWER 4 OF 7 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1994:568985 CAPLUS

DOCUMENT NUMBER: 121:168925

TITLE: Homoscorpionate (Tris(pyrazolyl)borate) Ligands

Containing Tethered 3-Phenyl Groups

AUTHOR(S): Rheingold, Arnold L.; Ostrander, Robert L.; Haggerty, Brian S.; Trofimenko, Swiatoslaw

CORPORATE SOURCE: Department of Chemistry, University of Delaware, Newark, DE, 19716-2522, USA

SOURCE: Inorg. Chem. (1994), 33(17), 3666-76

CODEN: INOCAJ; ISSN: 0020-1669

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Four new homoscorpionate ligands were prepd., 3 of them involving a 3-Ph substituent subject to steric control via tethering to the the 4-position of the pyrazole ring. The tethering prevents major departure from parallel alignment of the Ph and pyrazolyl rings. The choice of the tether (methylene or 1,2-ethylene) results in the Ph 6'-CH being either pulled away from the metal in the former case or thrust toward the metal in the latter. The effect of the 5-Me substituent on the bite of the ligand was also explored. The new ligands were hydrotris(2H-benz[g]-4,5-dihydroindazol-2-yl)borate (=Tpa), hydrotris(3-methyl-2H-benz[g]-4,5-dihydroindazol-2-yl)borate (=Tpa,Me), hydrotris(1,4-dihydroindeno[1,2-c]pyrazol-1-yl)borate (=Tpb), and hydrotris(3-phenyl-5-methylpyrazol-1-yl)borate (=Tpph,Me), each of which differed subtly in its coordinative behavior from the other 3. Complexes L2M, LMO, LRh(COD), LRh(CO)2, LRd(.eta.3-methallyl), and LMo(CO)2(.eta.3-methallyl) were synthesized, and the structures of TpaRh(CO)2, Tpa,MeZnI, TpbTl, and Tpph,MeZnI were detd. by x-ray crystallog. TpaRh(CO)2 crystallizes in the space group P.hivin.1, with a 8.574(2), b 20.113(6), c 20.188(6) .ANG., .alpha. 61.68(2), .beta. 84.14(2), .gamma. 85.15(2).degree. for Z = 4. Tpa,MeZnI crystallizes in the space group P212121, with a 10.002(1), b 16.237(3), c 19.952(3) .ANG. for Z = 4. TpbTl crystallizes in the space group P21/n, with a 11.363(2), b 11.096(2) .ANG., c 21.010(4) .ANG., .beta. 99.33(2).degree. for Z = 4. The Ph and pyrazolyl planes are essentially coplanar. Tpph,MeZnI crystallizes in the space group Pna21, with a 32.645(6), b 11.327(3), c 16.180(3) .ANG. for Z = 8. Cone and wedge angles were calcd. for the new ligands and compared with revised previously reported values.

IT 157409-94-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

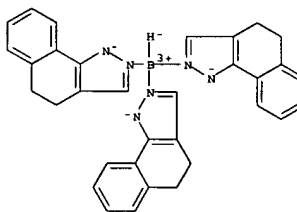
(prepn. of)

RN 157409-94-4 CAPLUS

CN Borate(1-), tris(4,5-dihydro-1H-benz[g]indazolato-.kappa.N2)hydro-, potassium, (T-4)- (9CI) (CA INDEX NAME)

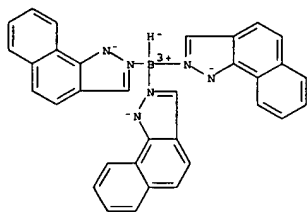
LB ANSWER 4 OF 7 CAPLUS COPYRIGHT 2002 ACS

(Continued)



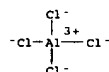
● K+

L8 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1994:701017 CAPLUS
 DOCUMENT NUMBER: 121:301017
 TITLE: A novel homoscorpionate ligand and its unusual bonding
 in a molybdenum complex
 AUTHOR(S): Rheingold, Arnold L.; Haggerty, Brian S.; Trofimenko, Swiatoslaw
 CORPORATE SOURCE: Dep. Chem., Univ. Delaware, Newark, DE, 19716-2522, USA
 SOURCE: J. Chem. Soc., Chem. Commun. (1994), (17), 1973-4
 CODEN: JCCCAT; ISSN: 0022-4936
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The new ligand, hydrotris(2H-benz[Glindazol-2-yl]borate, (L) forms octahedral and mixed octahedral [CoL2] and [CoL(L')] [L' = HB(3-neopentylpyrazolyl)]; an unusual complex [MoL(CO)2(.eta.3-CH2CMeCH2)], the structure of which is established by x-ray crystallog. shows L acting in a bidentate manner.
 IT 158989-18-5
 RL: RCT (Reactant)
 [a novel homoscorpionate ligand and its unusual bonding in a molybdenum complex]
 RN 158989-18-5 CAPLUS
 CN Borate(1-), tris(1H-benz[g]indazolato-.kappa.N2)hydro-, thallium(1+), (T-4)- (9CI) (CA INDEX NAME)

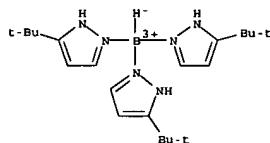


● Tl(I) +

L8 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



L8 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1994:579763 CAPLUS
 DOCUMENT NUMBER: 121:179763
 TITLE: Part I. Zinc and aluminum alkyl derivatives supported by oxygen and nitrogen ligation. Part II. The development of a structural and functional model for the enzyme carbonic anhydrase. Part III. A protonated tris(pyrazolyl)hydroborato ligand as an anion host
 AUTHOR(S): Looney, Adrian Gerard
 CORPORATE SOURCE: Columbia Univ., NY, USA
 SOURCE: (1993) 254 pp. Avail.: Univ. Microfilms Int., Order No. DA9412807
 From: Diss. Abstr. Int. B 1994, 54(12, Pt. 1), 6195
 Dissertation
 English
 DOCUMENT TYPE: English
 LANGUAGE: English
 AB Unavailable
 IT 135227-28-0
 RL: PRP (Properties)
 (structure of)
 RN 135227-28-0 CAPLUS
 CN Boron(2+), tris[5-(1,1-dimethylethyl)-1H-pyrazole-N2]hydro-, (T-4)-, chloride (T-4)-tetrachloroaluminate(1-) (9CI) (CA INDEX NAME)
 CM 1
 CRN 135227-27-9
 CMP C21 H37 B N6
 CCI CCS
 CDES 7:T-4



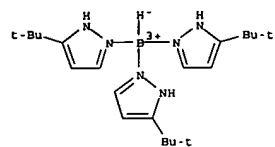
CM 2
 CRN 17611-22-2
 CMP Al Cl4
 CCI CCS
 CDES 7:T-4

L8 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1991:484035 CAPLUS
 DOCUMENT NUMBER: 115:84035
 TITLE: Anion coordination by protonated tris(pyrazolyl)hydroborato derivatives: crystal structure of the host-guest complex [(eta.3-HB(3-tert-Bu-pzH)3)Cl] [AlCl4]
 AUTHOR(S): Looney, Adrian; Parkin, Gerard; Rheingold, Arnold L.
 CORPORATE SOURCE: Dep. Chem., Columbia Univ., New York, NY, 10027, USA
 SOURCE: Inorg. Chem. (1991), 30(15), 3099-101
 CODEN: INOCAJ; ISSN: 0020-1669
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The mol. structure of the prepd. host-guest complex [(eta.3-HB(HR)3)Cl] [AlCl4] (R = 3-tert-Bu-pyrazolyl) was detd. by x-ray diffraction. The Cl- substrate is coordinated to the tris(pyrazolyl)hydroboronium host by 3 linear H bonds. 1.C6H6 is monoclinic, space group C2/c, a 25.144(5), b 10.246(2), c 29.420(5) .ANG., .beta. 101.40(1).degree., Z = 8, R = 0.0529, Rw = 0.0705.
 IT 135227-29-1P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and crystal structure of)
 RN 135227-29-1 CAPLUS
 CN Boron(2+), tris[5-(1,1-dimethylethyl)-1H-pyrazole-N2]hydro-, (T-4)-, chloride (T-4)-tetrachloroaluminate(1-), compd. with benzene (1:1) (9CI) (CA INDEX NAME)
 CM 1
 CRN 71-43-2
 CMP C6 H6



CM 2
 CRN 135227-28-0
 CMP C21 H37 B N6 . Al Cl4 . Cl
 CM 3
 CRN 135227-27-9
 CMP C21 H37 B N6
 CCI CCS
 CDES 7:T-4

L8 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2002 ACS (Continued)



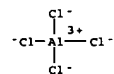
CM 4

CRN 17611-22-2

CMF A1 C14

CCI CCS

CDES 7:T-4




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L9          812 L3

=> s l9 and (metal or metals)
L10         290 L9 AND (METAL OR METALS)

=> s l10 and (lanthanide?)
L11         28 L10 AND (LANTHANIDE?)

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PROCESSING COMPLETED FOR L11
L12         28 DUP REM L11 (0 DUPLICATES REMOVED)

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PROCESSING COMPLETED FOR L11
L14         28 DUP REM L11 (0 DUPLICATES REMOVED)

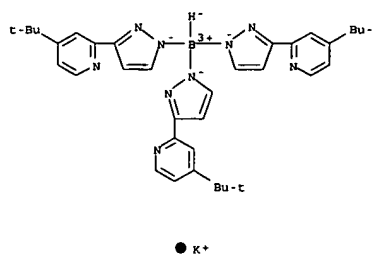
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YOU HAVE REQUESTED DATA FROM 28 ANSWERS - CONTINUE? Y/(N):y
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L14 ANSWER 1 OF 28 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2001:467040 CAPLUS
 DOCUMENT NUMBER: 135:282118
 TITLE: Syntheses and structures of lanthanide(III) complexes with some bis(pyrazolyl)borate and tris(pyrazolyl)borate podand ligands
 AUTHOR(S): Bell, Z. R.; Motson, G. R.; Jeffery, J. C.; McCleverty, J. A.; Ward, M. D.
 CORPORATE SOURCE: School of Chemistry, University of Bristol, Cantock's Close, Bristol, BS8 1TS, UK
 SOURCE: Polyhedron (2001), 20(15-16), 2045-2053
 CODEN: PLYHDE; ISSN: 0277-5387
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

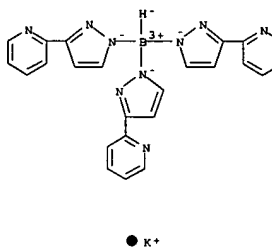
AB Two new poly(pyrazolyl)borate ligands were prepd.: potassium tris[3-((4-*t*-butyl)-pyrid-2-yl)-pyrazol-1-yl]hydroborate (KtpBuPy) which has three bidentate arms and is therefore hexadentate; and potassium bis[3-(2-pyridyl)-5-(methoxymethyl)pyrazol-1-yl]-dihydroborate (KBp(COC)Py) which has two bidentate arms and is therefore tetradentate. The crystal structures of their lanthanide complexes [La(TpBuPy)(NO₃)₂] and [La(Bp(COC)Py)₂](X⁻ = nitrate or triflate) were detd. In [La(TpBuPy)(NO₃)₂] the metal ion is ten-coordinate, from the hexadentate N-donor podand ligand and two bidentate nitrates. [La(Bp(COC)Py)₂(NO₃)₂] is also ten-coordinate, from two tetradentate ligands and a bidentate nitrate, but in [La(Bp(COC)Py)₂(CF₃SO₃)₂] the metal ion is nine-coordinate because the triflate anion is monodentate. Two unexpected new complexes which arose from partial decompn. of the poly(pyrazolyl)borate ligands also were characterized structurally. In [La(BuPy₂H)₃(O₃SCF₃)₃] the metal ion is nine-coordinate from three bidentate pyrazolyl-pyridine arms (liberated by decompn. of KtpBuPy) and three triflate anions; there is extensive NH...O hydrogen-bonding between the pyrazolyl and triflate ligands. [Nd(TpPy)(BpPy)] [Nd(Py₂H)(NO₃)₄] was isolated from the reaction of hexadentate tris[3-(2-pyridyl)-pyrazol-1-yl]hydroborate (TpPy) with Nd(NO₃)₃. One of the TpPy ligands has lost one bidentate pyrazolyl-pyridine 'arm' (Py₂H) to leave tetradentate tris[3-(2-pyridyl)-pyrazol-1-yl]dihydroborate (BpPy). In this structure, [Nd(TpPy)(BpPy)]⁺ is ten-coordinate from inter-leaved hexadentate and tetradentate ligands, and [Nd(Py₂H)(NO₃)₄]⁻ is also ten-coordinate from the bidentate N-donor ligand Py₂H and four bidentate nitrates.

IT 363594-39-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. and reactant for prepn. of lanthanum (pyridylpyrazolyl)borate and pyridylpyrazole complexes)
 RN 363594-39-2 CAPLUS
 CN Borate(1-), tris[4-(1,1-dimethylethyl)-2-(1H-pyrazol-3-yl)-.kappa.N1]pyridinato]hydro-, potassium, (T-4)- (9CI) (CA INDEX NAME)

L14 ANSWER 1 OF 28 CAPLUS COPYRIGHT 2002 ACS (Continued)



IT 161095-31-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reactant for prepn. of lanthanum (pyridylpyrazolyl)borate pyridylpyrazole complex)
 RN 161095-31-4 CAPLUS
 CN Borate(1-), hydrotris[2-(1H-pyrazol-3-yl)-.kappa.N1]pyridinato]-, potassium, (T-4)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L14 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2000:227727 CAPLUS
 DOCUMENT NUMBER: 132:271477
 TITLE: Divalent lanthanide metal complexes
 INVENTOR(S): Christou, Victor; Salata, Oleg Victorovich; Shipley, Christopher
 PATENT ASSIGNER(S): Isis Innovation Limited, UK
 SOURCE: PCT Int. Appl., 36 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

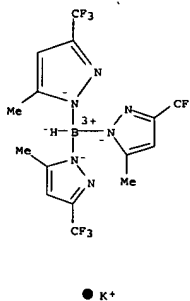
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000018851	A1	20000406	WO 1999-GB3201	19990924
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9961053	A1	20000417	AU 1999-61053	19990924
EP 1115808	A1	20010718	EP 1999-947674	19990924
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				

PRIORITY APPLN. INFO.: GB 1998-20805 A 19980925
 WO 1999-GB3201 W 19990924

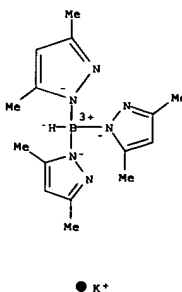
AB Light-emitting devices are described which employ complexes contg. a lanthanide (esp. Eu, Sm or Yb) cation complexed with 1 to 3 polydentate ligands. The polydentate ligands preferably contain 1H-pyrazol-1-yl groups, such as tris(1H-pyrazol-1-yl)borate anions. Selected complexes are claimed, as are methods for prepg. them by reacting the divalent cation with the complex ions in soln. and then sepg. the product from the soln.

IT 121314-30-5P
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (divalent lanthanide metal complexes with polydentate ligands and their prepn. and electroluminescent devices using them)
 RN 121314-30-5 CAPLUS
 CN Borate(1-), hydrotris[5-methyl-3-(trifluoromethyl)-1H-pyrazolato-.kappa.N1]-, potassium, (T-4)- (9CI) (CA INDEX NAME)

L14 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2002 ACS (Continued)

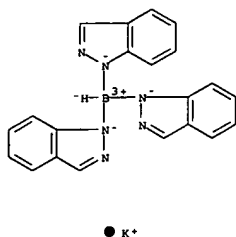


IT 17567-17-8 84768-84-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (divalent lanthanide metal complexes with polydentate ligands and their prepn. and electroluminescent devices using them)
 RN 17567-17-8 CAPLUS
 CN Borate(1-), tris(3,5-dimethyl-1H-pyrazolato-.kappa.N1)hydro-, potassium, (T-4)- (9CI) (CA INDEX NAME)



RN 84768-84-3 CAPLUS
 CN Borate(1-), hydrotris(1H-indazol-1-yl)-.kappa.N1]-, potassium, (T-4)- (9CI) (CA INDEX NAME)

L14 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2002 ACS (Continued)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
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L14 ANSWER 3 OF 28 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1999:720372 CAPLUS
DOCUMENT NUMBER: 132:72779
TITLE: Structural and Photophysical Properties of Mononuclear

AUTHOR(S):

Armaroli, Nicola; Accorsi, Gianluca; Serigelletti, Francesco; Couchman, Samantha M.; Fleming, James S.; Harden, Nicholas C.; Jeffery, John C.; Mann, Karen L. V.; McCleverty, Jon A.; Rees, Leigh H.; Starling, Sarah R.; Ward, Michael D.
CORPORATE SOURCE: Istituto di Fotochimica e Radiazioni d'Alta Energia del CNR, Bologna, 40129, Italy
SOURCE: Inorganic Chemistry (1999), 38(25), 5769-5776
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Lanthanide(III) complexes were prepd. with [L1]- [the tetradentate chelating ligand bis(3-(2-pyridyl)pyrazolyl)dihydroborate], [L2]- [the tetradentate chelating ligand bis(3-(2-pyrazolyl)pyrazolyl)dihydroborate], [L3]- [the hexadentate chelating ligand bis(3-(6'-(2,2'-bipyridyl))pyrazol-1-yl)dihydroborate], and [L4]- [the 12-dentate compartmental ligand hexakis(3-(2-pyridyl)pyrazol-1-yl)diboran(IV)ate, which has two hexadentate tris(pyrazolyl)borate-based cavities linked back-to-back by a B-B bond]. [Ln(L1)2(NO3)] are 10-coordinate with two tetradentate N-donor ligands and one bidentate nitrate. [Ln(L2)2(NO3)] have 10-coordinate structures similar to those

of the [L1]- complexes except that the coordinated N1 of the pyrazine rings is not such a good donor as the pyridine rings in the [L1]- complexes, leading to marked lengthening of these Ln-N bonds. [Ln(L3)2(NO3)2] are also 10-coordinate from one hexadentate chelating ligand which has a pseudoequatorial coordination mode and two pseudoaxial bidentate nitrate ligands; the hexadentate ligand has a shallow helical twist to prevent steric interference between its ends. Finally [Ln(NO3)2]2(L4)] are dinuclear, with each metal center being 10-coordinate from a tripodal hexadentate ligand cavity and two bidentate nitrates. Five complexes were structurally characterized: [Tb(L2)2(NO3)]·cndot.DMF is monoclinic (space group P21/c) with a 14.881(3), b 15.5199(12), c 15.845(2) .ANG., .beta. 92.387(12).degree., and Z = 4. [Gd(L2)2(NO3)]·cndot.DMF is monoclinic (space group P21/c) with a 14.926(2), b 15.465(2), c 15.878(2) .ANG., .beta. 92.698(11).degree., and Z = 4. [Eu(L3)2(NO3)2]·cndot.DMF·cndot.0.5Et2O is triclinic (P.hivin.1) with a 10.020(3), b 13.036(3), c 14.740(3) .ANG., .alpha. 70.114(14), .beta. 71.55(2), .gamma. 79.66(2).degree., and Z = 2. [[La(NO3)2(DMF)2]2(L4)]·cndot.DMF is orthorhombic (Pbca) with a 18.813(2), b 15.241(2), c 27.322(2) .ANG., and Z = 4. [[Gd(NO3)2]2(L4)]·cndot.2.4DMF is tetragonal (P42/n) with a 16.632(6), c 24.19(5) .ANG., and Z = 4. Detailed photophys. studies were performed on the free ligands and their complexes with Gd(III), Eu(III), and Tb(III)

in several solvents. The results show a wide range in the emission properties of the complexes which can be rationalized in terms of subtle variations in the steric and electronic properties of the ligands. In

L14 ANSWER 3 OF 28 CAPLUS COPYRIGHT 2002 ACS (Continued)
particular the dinuclear Tb(III) complex of [L4]2- has an emission quantum yield of .apprx.0.5 in D2O and MeOD.

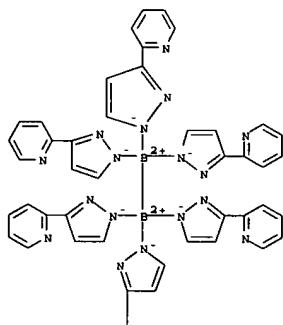
IT 212397-25-6

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(complexation with lanthanide(III) and photophys. properties of)

RN 212397-25-6 CAPLUS

CN Diborate(2-), hexakis[2-(1H-pyrazol-3-yl-.kappa.N1)pyridinato]-, dipotassium (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L14 ANSWER 4 OF 28 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1999:446779 CAPLUS
DOCUMENT NUMBER: 131:178534
TITLE: Syntheses of new [tetrakis(1-pyrazolyl)borato]samarium(III) complexes and their temperature-dependent exchange motions of all pyrazolyl groups

AUTHOR(S):

Onishi, Masayoshi; Yamaguchi, Hitoshi; Shimotsu, Hirokazu; Hiraki, Katsuma; Nageoka, Junko; Kawano, Hiroyuki
CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering, Nagasaki University, Nagasaki, 852-8521, Japan

SOURCE:

Chemistry Letters (1999), (7), 573-574
CODEN: CHLTAG; ISSN: 0366-7022
PUBLISHER: Chemical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English

AB As the 1st unambiguous syntheses and characterization of the [tetrakis(1-pyrazolyl)borato]lanthanide(III) complexes, stable eight-coordinate [Ln(beta.-ketoenolato)4]samarium [Sm{eta.3-B(pz)4}2(beta.-

ketoenolato)] (pz = 1-pyrazolyl group; .beta.-ketoenolato = acetylacetonato, salicylaldehyde, 2,2,6,6-tetramethylheptane-3,5-dione, 3-methylpentane-2,4-dione) were prepd., and novel stereochem. nonrigid temp.-dependent motions of the B(pz)4 ligands were obsd. on their

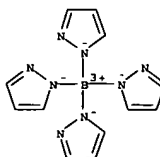
soln.-state 1H-NMR spectra, showing the spectroscopic equivalence of coordinated and uncoordinated pyrazolyl groups at high temps.

IT

RL: RCT (Reactant); RACT (Reactant or reagent)
(for prepn. of samarium tetrakis(pyrazolyl)borato ketoenolato complexes)

RN 14782-58-2 CAPLUS

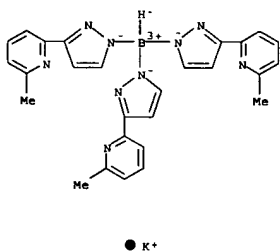
CN Borate(1-), tetrakis(1H-pyrazolato-.kappa.N1)-, potassium (9CI) (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L14 ANSWER 4 OF 28 CAPLUS COPYRIGHT 2002 ACS (Continued)

L14 ANSWER 5 OF 28 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1999:55807 CAPLUS
 DOCUMENT NUMBER: 130:245582
 TITLE: Lanthanide complexes of a new sterically hindered potentially hexadentate podand ligand based on a tris(pyrazolyl)borate core; crystal structures, solution structures and luminescence properties
 AUTHOR(S): Reeves, Zoe R.; Mann, Karen L. V.; Jeffery, John C.; McCleverty, Jon A.; Ward, Michael D.; Barigelli, Francesco; Armaroli, Nicola
 CORPORATE SOURCE: School of Chemistry, University of Bristol, Bristol, BS8 1TS, UK
 SOURCE: Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1999), (3), 349-356
 CODEN: JCDTBI; ISSN: 0300-9246
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The new podand ligand hydrotris[3-(6-methylpyridin-2-yl)pyrazol-1-yl]borate [L1]- was prepd. which contains three bidentate pyrazolyl/pyridine arms attached to a [BH]- head-group. This ligand differs from an earlier ligand hydrotris[3-(2-pyridyl)pyrazol-1-yl]borate [L2]- by the presence of Me groups attached to the C6 positions of the pyridyl rings, which would interfere with each other sterically if the ligand coordinated in a fully hexadentate manner. Instead, crystallog. anal. of [M(L1)(NO3)2(H2O)] (M = Eu, Tb or Gd) showed that partial disocn. of the podand occurs to relieve this potential steric problem: either one or two of the pyridyl groups are not coordinated, such that [L1]- is penta- or tetra-dentate, but instead are involved in intramol. N.cntdot..cntdot..cntdot.H-O hydrogen-bonding interactions with the coordinated water mol. The presence of both structural forms in single crystals of the gadolinium and europium complexes shows that interconversion between them in soln. must be facile. Variable-temp. 1H NMR spectra of the diamagnetic lanthanum(III) analog shows that, whereas all three ligand arms are equiv. on the NMR timescale at high temps., at -80.degree. there is mirror symmetry in the complex such that two arms are equiv. and the 3rd is different from the other two; this is consistent with the cryst. form in which [L1]- is tetradentate with two pendant pyridyl arms, which has pseudo-mirror symmetry. Luminescence studies showed that whereas the ligand-based luminescence is retained in the gadolinium(III) complex, in the europium(III) and terbium(III) complexes the ligand-centered emission is quenched by ligand-to-metal energy transfer, resulting in the usual metal-centered emission spectra. The intensity of the emission from the europium(III) and terbium(III) complexes of [L1]- is substantially reduced compared to the emission from the analogous complexes [M(L2)(NO3)2] (M = Eu or Tb) which the authors ascribe to the sterically induced poorer coordination of the podand ligand, resulting in (i) less efficient ligand-to-metal energy transfer, and (ii) coordination of labile solvent mols. (H2O) to the metal centers.
 IT 221367-97-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (prepn. and complexation with rare earths)
 RN 221367-97-1 CAPLUS
 CN Borate(1-), hydrotris[2-methyl-6-(1H-pyrazol-3-yl)-kappa.N1]pyridinato]-,

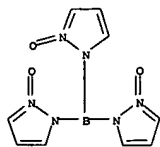
L14 ANSWER 5 OF 28 CAPLUS COPYRIGHT 2002 ACS (Continued)
potassium (9CI) (CA INDEX NAME)

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L14 ANSWER 6 OF 28 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1999:9912 CAPLUS
 DOCUMENT NUMBER: 130:102684
 TITLE: Electroluminescent material
 INVENTOR(S): Kathirgamanathan, Poopathy
 PATENT ASSIGNEE(S): South Bank University Enterprises Ltd., UK
 SOURCE: PCT Int. Appl., 39 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9858037	A1	19981223	WO 1998-GB1773	19980617
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CP, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
AU 9881165	A1	19990104	AU 1998-81165	19980617
AU 741025	B2	20011122		
EP 990016	A1	20000405	EP 1998-930877	19980617
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI			
JP 2002505701	T2	20020219	JP 1999-503979	19980617
PRIORITY APPLN. INFO.:			GB 1997-12483	A 19970617
			WO 1998-GB1773	W 19980617
OTHER SOURCE(S):			MARPAT 130:102684	
AB	Electroluminescent devices comprising a transparent substrate on which is formed a layer of an electroluminescent material are described in which the electroluminescent material is a rare earth metal, actinide or transition metal org. complex which has a photoluminescent efficiency (PL) >25%, preferably >40%. Electroluminescent complexes are also described, in which the metal is a rare earth, transition metal, lanthanide, or an actinide and gtoreq.1 of the ligands is either O-C(R')-C(R'')-O or a 2,2'-Bis(pyridyl)ketone deriv. (R' = (un)substituted arom. or heterocyclic ring structures, a hydrocarbyl of a fluorocarbon, or tert-butyl; and R'' = (un)substituted arom. or heterocyclic ring structures, a hydrocarbyl of a fluorocarbon, P, or H, or can be part of a copolymer). Preferably, the metals are selected from Sm(III), Eu(III), Tb(III), Dy(III), Yb(III), Lu(III), Gd(III), Eu(II), U(III), UO2(VI), and Th(III).			
IT	219121-79-6D, terbium dipivaloylmethane complexes RL: DEV (Device component use); USES (Uses) (electroluminescent materials based on metal complexes and devices using them)			
RN	219121-79-6 CAPLUS			
CN	1H-Pyrazole, 1,1',1''-borylidymetris-, 2,2',2''-trioxide (9CI) (CA INDEX NAME)			

L14 ANSWER 6 OF 28 CAPLUS COPYRIGHT 2002 ACS (Continued)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

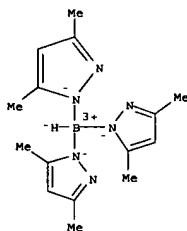
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L14 ANSWER 7 OF 28 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1998:806731 CAPLUS
 DOCUMENT NUMBER: 130:73617
 TITLE: Organometallic complexes
 INVENTOR(S): Christou, Victor
 PATENT ASSIGNEE(S): Isis Innovation Ltd., UK
 SOURCE: PCT Int. Appl., 38 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

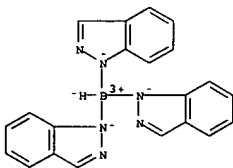
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9855561	A1	19981210	WO 1998-GB1587	19980601
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, BG, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
AU 9876681	A1	19981221	AU 1998-76681	19980601
EP 988353	A1	20000329	EP 1998-924488	19980601
R:	BE, DE, ES, FR, GB, IT, NL			
JP 2002513440	T2	20020508	JP 1999-501831	19980601
PRIORITY APPLN. INFO.:			GB 1997-11237	A 19970602
			WO 1998-GB1587	W 19980601

OTHER SOURCE(S): MARPAT 130:73617
 AB Light-emitting devices are described which employ organometallic complexes comprising a lanthanide metal cation complexed with 1-3 polydentate ligands contg. .gtoreq.1 (un)substituted pyrazolyl groups optionally fused with (un)substituted heterocyclic or carbocyclic (non)arom. ring systems, with a coordinate bond formed between the metal and one of the nitrogen atoms of the pyrazolyl rings. Preferably, the ligands comprise trispyrazolyl borate deriva. Organometallic compds. suitable for the devices are also claimed, as are methods of producing them entailing the reaction of the ligands with a cation followed by sepn. of the products. Compns. combining the compds. with a matrix material are also described. Use in electroluminescent flat panel displays is also described.
 IT 17567-17-8 84768-84-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (lanthanide-pyrazolyl deriv. complexes and electroluminescent devices and displays using them)
 RN 17567-17-8 CAPLUS
 CN Borate(1-), tris(3,5-dimethyl-1H-pyrazolato-.kappa.N1)hydro-, potassium, (T-4)- (9CI) (CA INDEX NAME)

L14 ANSWER 7 OF 28 CAPLUS COPYRIGHT 2002 ACS (Continued)

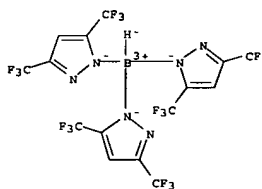
● K⁺

RN 84768-84-3 CAPLUS
 CN Borate(1-), hydrotris(1H-indazolato-.kappa.N1)-, potassium, (T-4)- (9CI) (CA INDEX NAME)

● K⁺

IT 167898-36-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (lanthanide-pyrazolyl deriv. complexes and electroluminescent devices and displays using them)
 RN 167898-36-4 CAPLUS
 CN Borate(1-), tris[3,5-bis(trifluoromethyl)-1H-pyrazolato-.kappa.N1]hydro-, potassium, (T-4)- (9CI) (CA INDEX NAME)

L14 ANSWER 7 OF 28 CAPLUS COPYRIGHT 2002 ACS (Continued)

● K⁺

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L14 ANSWER 8 OF 28 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1998:577455 CAPLUS

DOCUMENT NUMBER: 129:239129

TITLE: Heterodinuclear Complexes Containing d- and f-block Elements: Synthesis, Structural Characterization, and Metal-Metal Interactions of Novel Chromium(III)-Lanthanide(III) Compounds Bridged by Oxalate

AUTHOR(S): Sanada, Takayuki; Suzuki, Takayoshi; Yoshida, Takafumi; Kaizaki, Sumio

CORPORATE SOURCE: Department of Chemistry Graduate School of Science, Osaka University, Toyonaka, 560, Japan

SOURCE: Inorganic Chemistry (1998), 37(18), 4712-4717

CODEN: INOCAJ; ISSN: 0020-1669

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The reaction of Ln(III) ions with a tripodal ligand HBpz3- (hydrotris(pyrazol-1-yl)borate) and a complex ligand [Cr(acac)2(ox)]- (acac- = acetylacetonate, ox2- = oxalate) in aq. soln. afforded the novel 3d-4f heterodinuclear complexes [(acac)2Cr(ox)Ln(HBpz3)2] (Ln = Eu (1),

Gd (2), Tb (3), Yb (4), Lu (5)). 4 Crystallizes in monoclinic space group P2₁/n, with a 8.594(3), b 18.538(4), c 12.093(2) .ANG., .beta. 93.71(2).degree., and Z = 2. Yb coordinates in an eight-coordinate distorted square antiprismatic geometry. The intramol. Cr..cntdot..cntdot..cntdot.Yb distance is 5.631(1) .ANG.. The magnetic susceptibility data for 2 showed that the Cr(III)-Gd(III) interaction is weakly antiferromagnetic with an exchange coupling const. JCrGd = -0.09 cm-1. The luminescence measurements demonstrated the energy transfers

for both Ln(III) .fwdarw. Cr(III) and Cr(III) .fwdarw. Ln(III), of which the degree of emission quenching depends on the energy gap of the excited levels in two metal centers. These results reveal that the metal-metal interactions between Cr(III) and Ln(III) are very weak in magnetic interaction but are strong from the viewpoint of energy transfer.

IT 18583-60-3, Potassium hydrotris(pyrazol-1-yl)borate

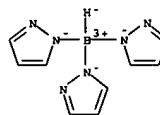
RL: RCT (Reactant); RACT (Reactant or reagent)

(complexation with rare earth ions)

RN 18583-60-3 CAPLUS

CN Borate(1-), hydrotris(1H-pyrazolato-.kappa.N1)-, potassium, (T-4)- (9CI) (CA INDEX NAME)

L14 ANSWER 8 OF 28 CAPLUS COPYRIGHT 2002 ACS (Continued)

● K⁺

L14 ANSWER 9 OF 28 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1999:95535 CAPLUS

DOCUMENT NUMBER: 130:217132

TITLE: Chloro-lanthanide, and plutonium complexes containing the hydrotris(3,5-dimethylpyrazol-1-yl)borate ligand: the crystal and molecular

structures of [PrCl(.mu.-Cl)TpMe2(3,5-Me2pzH)]2 and YbCl2TpMe2(THF)

AUTHOR(S): Apostolidis, C.; Carvalho, A.; Domingos, A.;

Kanellakopulos, B.; Maier, R.; Marques, N.; De Matos, A. Pires; Rebizant, J.

CORPORATE SOURCE: European Commission, Joint Research Centre, Institute for Transuranium Elements, Karlsruhe, D-76725,

Germany

SOURCE: Polyhedron (1998), Volume Date 1999, 18(1-2), 263-272

CODEN: PLYHDE; ISSN: 0277-5387

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Reactions of PuCl3 and LnCl3 (Ln = Pr, Nd) with the stoichiometric amt. of

KTpMe2 (TpMe2 = HB(3,5-Me2pz)3) yielded the dimeric [MCl(.mu.-Cl)TpMe2(Me2pzH)]2 compds. (M = Pu (1), Pr (2), Nd (3)). The analogous reaction with YbCl3 afforded the monomeric YbCl2TpMe2(THF) complex (4). The crystal and mol. structures of 2 and 4 were assessed by single

crystal X-ray diffraction anal. In 2 each Pr atom is seven-coordinate and is linked to the adjacent metal center by two bridging Cl ligands. In 4 the Yb atom is six-coordinate and displays octahedral geometry. 4 Undergoes intermol. rearrangement reactions to yield [YbCl2TpMe2(Me2pzH)]..cntdot..THF (6) and [YbCl3TpMe2]-(Me2pzH2))+ (7). The mol. structures of 6 and 7 were detd. by x-ray diffraction. In 6 the tridentate ligand, the two Cl atoms and the N atom of the neutral dimethylpyrazole describe a distorted octahedron. 7 Consists of discrete [YbCl3TpMe2]- and [(Me2pzH2)]+ ions, with the Yb atom of the cation coordinated to three pyrazolyl nitrogens and three Cl atoms.

IT 17567-17-8 142198-03-6

RL: RCT (Reactant); RACT (Reactant or reagent)

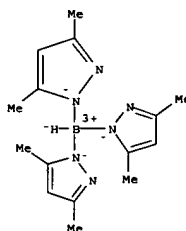
(for prepn. of rare earth hydrotris(pyrazolyl)borate complexes)

RN 17567-17-8 CAPLUS

CN Borate(1-), tris(3,5-dimethyl-1H-pyrazolato-.kappa.N1)hydro-, potassium,

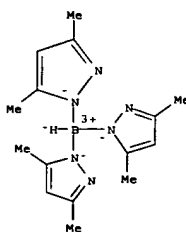
(T-4)- (9CI) (CA INDEX NAME)

L14 ANSWER 9 OF 28 CAPLUS COPYRIGHT 2002 ACS (Continued)

● K⁺

RN 142198-03-6 CAPLUS

CN Borate(1-), tris(3,5-dimethyl-1H-pyrazolato-.kappa.N1)hydro-, sodium, (T-4)- (9CI) (CA INDEX NAME)

● Na⁺

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L14 ANSWER 10 OF 28 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1997:436063 CAPLUS
 DOCUMENT NUMBER: 127:51112
 TITLE: Olefin polymerization catalysts based on metal complexes
 INVENTOR(S): Jens, Klaus Joachim; Tilset, Mats; Heuman, Andreas
 PATENT ASSIGNEE(S): Borealis A.S. Norway; Cockbain, Julian; Jens, Klaus Joachim; Tilset, Mats; Heuman, Andreas
 SOURCE: PCT Int. Appl., 45 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9717379	A1	19970515	WO 1996-GB2743	19961108
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TW				
RW: KE, LS, MM, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BP, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9675024	A1	19970529	AU 1996-75024	19961108
PRIORITY APPLN. INFO.: GB 1995-22859 19951108 WO 1996-GB2743 19961108				

OTHER SOURCE(S): MARPAT 127:51112
 AB The invention provides a novel olefin polymn. catalyst, in particular an olefin polymn. catalyst compd. comprising a catalytically effective transition metal, lanthanide, or actinide complexed by a pyrazol-1-yl group contg. complexant, characterized in that said complexant contains a pyrazol-1-yl group substituted in the 3-position by an org. moiety contg. at least 3 carbon atoms. This catalyst provides good control of the mol. wt. and mol.-wt. distribution of the polymers.

A typical catalyst was manufd. by reaction of TiCl_4 with K hydrottris(5-methyl-3-phenylpyrazol-1-yl)borate.
 IT 106209-98-7P 185034-21-3P
 RL: IMP (Industrial manufacture); RCT (Reactant); PREP (Preparation);
 RACT (Reactant or reagent)
 (catalyst precursor; olefin polymn. catalysts based on metal complexes contg. 3-substituted pyrazoles)
 RN 106209-98-7 CAPLUS
 CN Borate(1-), hydrottris(3-phenyl-1H-pyrazolato-.kappa.N1)-, potassium, (T-4)- (9CI) (CA INDEX NAME)

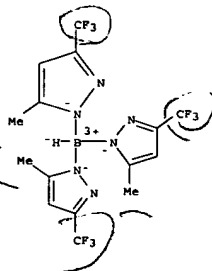
L14 ANSWER 11 OF 28 USPATFULL

ACCESSION NUMBER: 97:38507 USPATFULL
 TITLE: Pyrazolyl borates complexes-(IAW294)
 INVENTOR(S): Gorun, Sergiu M., Upper Montclair, NJ, United States
 Stribany, Robert T., Long Valley, NJ, United States
 EXXON Research and Engineering Company, Florham Park, NJ, United States (U.S. corporation)

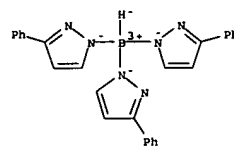
NUMBER	KIND	DATE
PATENT INFORMATION:	US 5627164	19970506
APPLICATION INFO.:	US 1995-489860	19950613 (8)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	Granted	
PRIMARY EXAMINER:	McKane, Joseph K.	
LEGAL REPRESENTATIVE:	Dvorak, Joseph J.	
NUMBER OF CLAIMS:	9	
EXEMPLARY CLAIM:	1	
NUMBER OF DRAWINGS:	2 Drawing Figure(s); 2 Drawing Page(s)	
LINE COUNT:	192	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
 AB Briefly stated, the present invention comprises a composition of matter having the formula $\text{M.sub.x.L.sub.y.P.sub.z.nQ}$ where M is a metal, P is a counterion, x, y, and z are integers, Q is a solvent, n is a numerical value of from 0 to about 12, and L is either a tris or a bis substituted pyrazolyl borate anion having the structural formula:
 #STR1#

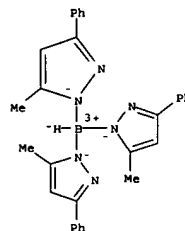
IT 121314-30-5 (for prepn. of trifluoromethyl-substituted tris(pyrazolyl)borate metal complex)
 RN 121314-30-5 USPATFULL
 CN Borate(1-), hydrottris(5-methyl-3-(trifluoromethyl)-1H-pyrazolato-.kappa.N1)-, potassium, (T-4)- (9CI) (CA INDEX NAME)

● K⁺

L14 ANSWER 10 OF 28 CAPLUS COPYRIGHT 2002 ACS (Continued)

● K⁺

RN 185034-21-3 CAPLUS
 CN Borate(1-), hydrottris(5-methyl-3-phenyl-1H-pyrazolato-.kappa.N1)-, potassium, (T-4)- (9CI) (CA INDEX NAME)

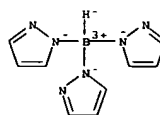
● K⁺

L14 ANSWER 12 OF 28 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1997:117153 CAPLUS
 DOCUMENT NUMBER: 126:194462
 TITLE: Homoscorpionates (hydrottris(1-pyrazolyl)borato complexes) of the trivalent 4f ions. The crystal and molecular structure of $[\text{HB}(\text{N}2\text{C}3\text{H}3)3]3\text{LnIII}$, (Ln = Pr, Nd)
 AUTHOR(S): Apostolidis, C.; Rebizant, J.; Kanellakopoulos, B.; von Ammon, R.; Dornberger, E.; Mueller, J.; Powietzka, B.; Nuber, B.
 CORPORATE SOURCE: Inst. Transuranium Elements, European Commission, Karlsruhe, D-76125, Germany
 SOURCE: Polyhedron (1997), 16(7), 1057-1068
 CODEN: PLYHDE; ISSN: 0277-5387
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The complexes $[\text{eta}^3\text{-HB}(\text{N}2\text{C}3\text{H}3)3]3\text{M}$ ($\text{N}2\text{C}3\text{H}3$ = hydrottris(1-pyrazolyl)borato = Tp) of scandium, yttrium, lanthanum and of the trivalent lanthanides from cerium to lutetium (with the exception of promethium) were synthesized by the reaction of MCl_3 with $\text{K}[\text{HB}(\text{N}2\text{C}3\text{H}3)3]$ in THF or in water. The crystal and mol. structures of the Pr and Nd compds. were detd. by single-crystal x-ray diffraction. The crystal structure corresponds to the structure of the praseodymium trichloride (LaCl_3 -type). The Pr^{3+} is nine-coordinate to the N atoms of the three Tp ligands. One N atom of each of the three Tp ligands and the Pr ion are almost coplanar with a Pr-N distance of 278.3 pm, while all of the other six N atoms are at a distance of 269.9 pm in a tricapped trigonal prismatic arrangement. The M-N distances in the Nd compd. are 280.4 (3x) and 259.9 (6x) pm. IR spectroscopic studies showed that the metal ion in the LnTp_3 compds. from La to Dy is nine-coordinate, while in the compds. of the heavier lanthanides from Ho to Lu, and Sc and Y, the central ion is eight-coordinate.

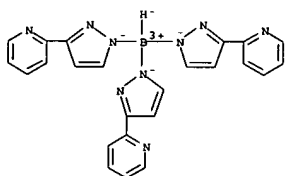
IT 18583-60-3, Potassium hydrottris(1-pyrazolyl)borate
 RL: RCT (Reactant)
 (for prepn. of rare earth and group IIIB metal hydrottris(pyrazolyl)borato complexes)
 RN 18583-60-3 CAPLUS
 CN Borate(1-), hydrottris(1H-pyrazolato-.kappa.N1)-, potassium, (T-4)- (9CI) (CA INDEX NAME)

● K⁺

L14 ANSWER 12 OF 28 CAPLUS COPYRIGHT 2002 ACS (Continued)

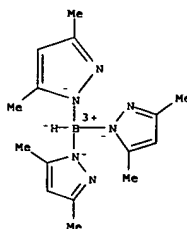
L14 ANSWER 13 OF 28 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1996:734439 CAPLUS
 DOCUMENT NUMBER: 126:69292
 TITLE: Lanthanide Complexes of the Hexadentate N-donor Podand
 Tris[3-(2-pyridyl)pyrazolyl]hydroborate
 : Solid-State and Solution Properties
 AUTHOR(S): Jones, Peter L.; Amoroso, Angelo J.; Jeffery, John C.; McCleverty, Jon A.; Psillakis, Eleftheria; Rees, Leigh H.; Ward, Michael D.
 CORPORATE SOURCE: School of Chemistry, University of Bristol, Bristol, BS8 1TS, UK
 SOURCE: Inorganic Chemistry (1997), 36(1), 10-18
 CODEN: INOCAJ; ISSN: 0020-1669
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The hexadentate N6-donor podand tris[3-(2-pyridyl)pyrazolyl]hydroborate (TpPy) contains 2-pyridyl fragments attached to the pyrazolyl C3-positions such that each arm is a bidentate chelate. Three series of lanthanide(III) complexes were prepd.: [M(TpPy)(MeOH)2][PF6] (series A), [M(TpPy)(NO3)2] (series B), and [M(TpPy)2][BPh4] (series C). Crystallog. studies showed that series A and B have a 1:1 metal :TpPy ratio, with the metal ion lying within the podand cavity and the remaining coordination sites occupied by solvent mols. and/or counterions to give 9-coordination (A, with one fluoride and two MeOH ligands) or 10-coordination (B, with two bidentate nitrate-ligands). The C complexes were prepd. in the absence of any coordinating anions and have a 1:2 metal:TpPy ratio with an unusual icosahedral geometry arising from coordination of the 12 N donors from two interleaved podands. Soln. cond. studies on the B complexes show that in H2O the nitrates dissociate to give [M(TpPy)(H2O)q](NO3)2; the relaxivity of [Gd(TpPy)(NO3)2] in H2O is 4.4 s-1 mM-1, a value comparable to those of clin. useful MRI contrast enhancement agents. Comparison of emission lifetimes of [M(TpPy)(NO3)2] (M = Eu, Tb) in H2O/D2O and MeOH/CD3OD give values for q, the no. of coordinated solvent mols., of 3.6 (water) and 2.6 (MeOH). The C complex [Tb(TpPy)2][BPh4] also has q = 2.6 in MeOH, suggesting that partial ligand dissociation allows access of solvent mols. to the metal coordination sphere.
 IT 161095-31-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (for prepn. of lanthanide tris[3-(2-pyridyl)pyrazolyl]hydroborate complexes)
 RN 161095-31-4 CAPLUS
 CN Borate(1-), hydrotris[2-(1H-pyrazol-3-yl)-kappa.N1]pyridinato]-, potassium, (T-4) - (9CI) (CA INDEX NAME)

L14 ANSWER 13 OF 28 CAPLUS COPYRIGHT 2002 ACS (Continued)



● K+

L14 ANSWER 14 OF 28 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1996:689344 CAPLUS
 DOCUMENT NUMBER: 126:31698
 TITLE: A Catalytic System for Ethylene Polymerization Based on Group III and Lanthanide Complexes of Tris(pyrazolyl)borate Ligands
 AUTHOR(S): Long, David P.; Bianconi, Patricia A.
 CORPORATE SOURCE: Department of Chemistry, Pennsylvania State University, University Park, PA, 16802, USA
 SOURCE: Journal of the American Chemical Society (1996), 118(49), 12453-12454
 CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Numerous reports have shown the viability of tris(pyrazolyl)borates as an effective ligand system for the system control around a metal center. WE report here the synthesis and characterization of tris(3,5-dimethyl-1-pyrazolyl)borohydride (TpMe) complexes of yttrium of the general formula [YpMeR2(THF)x] [R = C6H5, CH2SiMe3]. We have found these complexes and similar ones of variously substituted Tp ligands, as well as analogous lanthanide complexes, to be active in the catalytic polymn. of ethylene to linear, extremely high mol. wt. polymers. The variations in polymn. activity and yields of polyethylene (PE) that are obtained from different members of this class of complexes show that synthetic tailoring allows control over the rate of the polymn. reaction and the yield of the PE product.
 IT 17567-17-8, Potassium hydridotris(3,5-dimethylpyrazolyl)borate(1-)
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (catalyst prepn.; prepn. of a catalytic system for ethylene polymn. based on group III and lanthanide complexes of tris(pyrazolyl)borate ligands)
 RN 17567-17-8 CAPLUS
 CN Borate(1-), tris(3,5-dimethyl-1H-pyrazolato-kappa.N1)hydro-, potassium, (T-4) - (9CI) (CA INDEX NAME)

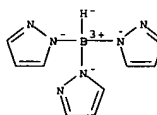


● K+

L14 ANSWER 14 OF 28 CAPLUS COPYRIGHT 2002 ACS (Continued)

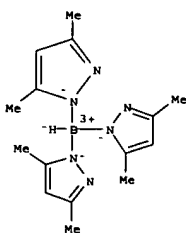
L14 ANSWER 15 OF 28 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:125920 CAPLUS
DOCUMENT NUMBER: 124:248762
TITLE: Heteroleptic poly(pyrazolyl)borate derivatives of the lanthanides. Structural and electronic spectral studies of some salicylaldehyde complexes
AUTHOR(S): Lawrence, Royston G.; Jones, Christopher J.; Kresinski, Roman A.
CORPORATE SOURCE: Sch. Chem., Univ. Birmingham, Birmingham, B15 2TT, UK
SOURCE: J. Chem. Soc., Dalton Trans. (1996), (4), 501-7
CODEN: JCDTBI; ISSN: 0300-9246
DOCUMENT TYPE: Journal
LANGUAGE: English
AB [Ln(HB(pz)3)2L] (pz = pyrazol-1-yl; L = salicylaldehyde, Ln = Y, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Yb or Lu; L = 5-methoxysalicylaldehyde (mosal), Ln = Y, Pr, Nd, Sm, Eu, Gd, Tb, Yb or Lu) were synthesized and the crystal structure of [Eu(HB(pz)3)2(mosal)] detd. The Eu ion is eight-coordinate with Eu-O distances of 2.266(5) and 2.402(5) Å. polytopal anal. indicates that the coordination geometry is best described as dodecahedral. The solid-angle sum of 0.768 is close to the norm for eight-coordinate. These structural parameters were compared with those calcd. for the previously reported binuclear complex {[Sm(HB(pz)3)2(O2CPh)]2} and estd. for its monomeric counterpart, which is as yet unknown. The use of such data in predicting when complexes of this type will dimerize was assessed. Electronic spectra of the Nd complexes revealed <1% covalency in the metal-ligand bonding and emission spectral data are reported for the Eu and Tb complexes.
IT 18583-60-3 Potassium hydrotris(1-pyrazolyl)borate
RL: RCT (Reactant)
RN 18583-60-3 CAPLUS
CN Borate(1-), hydrotris(1H-pyrazolato- κ .N1)-, potassium, (T-4)- (9CI) (CA INDEX NAME)

● K⁺

L14 ANSWER 16 OF 28 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1995:983008 CAPLUS
DOCUMENT NUMBER: 124:44142
TITLE: Synthesis and Molecular Structures of Hydrotris(dimethylpyrazolyl)borate Complexes of the Lanthanides
AUTHOR(S): Liu, Sung-Ying; Maunders, Graham H.; Sella, Andrea; Stevenson, Maya; Tocher, Derek A.
CORPORATE SOURCE: Department of Chemistry, UCL, London, WC1H 0AJ, UK
SOURCE: Inorg. Chem. (1996), 35(1), 76-81
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The reaction of lanthanide triflates with 2 equiv of K hydrotris(3,5-dimethylpyrazolyl)borate (TpMe2) gives good yields of complexes Ln(TpMe2)2OTf. For La (2), Ce (3), Pr (4), and Nd (5) the complexes are seven-coordinate in the solid state with the triflate group coordinated to the metal in unidentate fashion. Complex 5 crystallizes in the monoclinic space group P21/c with a 17.629(3), b 12.740(2), c 18.163(3) Å, β 107.35(1)°, Z = 4, and R_w = 0.0458. For the complexes of Y (1), Sm (6), Eu (7), Gd (8), Dy (9), Ho (10), and Yb (11), the smaller size of the metal ion leads to ejection of the triflate from the coordination sphere and the complexes are ionic in the solid state with a six-coordinate metal center. Complex 11 crystallizes in the monoclinic space group C2/m with a 16.593(7), b 13.671(5), c 8.746(2) Å, β 91.66(3)°, Z = 2, and R_w = 0.0416. In soln., however, complex 6 adopts a seven-coordinate mol. structure with the triflate ion within the 1st coordination sphere.
IT 17567-17-8 Potassium hydrotris(3,5-dimethylpyrazolyl)borate
RL: RCT (Reactant)
RN 17567-17-8 CAPLUS
CN Borate(1-), tris(3,5-dimethyl-1H-pyrazolato- κ .N1)hydro-, potassium, (T-4)- (9CI) (CA INDEX NAME)

● K⁺

L14 ANSWER 17 OF 28 USPATFULL

ACCESSION NUMBER: 95:66935 USPATFULL
TITLE: Fluorescent compounds
INVENTOR(S): Bell, Colin D., Cardiff, United Kingdom
Hovess, John H. C., Cardiff, United Kingdom
PATENT ASSIGNEE(S): Amersham International plc, United Kingdom (non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 5435937		19950725
APPLICATION INFO.:	US 1993-17674		19930212 (8)

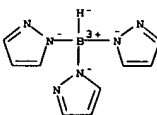
	NUMBER	DATE
PRIORITY INFORMATION:	EP 1992-301249	19920214
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	Granted	
PRIMARY EXAMINER:	Willis, Jr., Prince	
ASSISTANT EXAMINER:	Diamond, Alan D.	
LEGAL REPRESENTATIVE:	Wenderoth, Lind & Ponack	
NUMBER OF CLAIMS:	28	
EXEMPLARY CLAIM:	1	
NUMBER OF DRAWINGS:	12 Drawing Figure(s); 10 Drawing Page(s)	
LINE COUNT:	1046	
CAS INDEXING IS AVAILABLE FOR THIS PATENT.		

AB Novel compounds obtainable by reacting together an imido-reagent such as

diphenylphosphonimidoditriphenylphosphorane) with a chelate of a transition or lanthanide or actinide metal, such as tris(dibenzoylmethide) europium III, has the property of fluorescing in UV radiation. The invention includes solid polymer bodies containing such compounds, or chelates of transition or lanthanide or actinide metals generally, the bodies having the property of emitting light by virtue of internally generated, e.g. by tritium ionising radiation. The body is preferably of polystyrene formed by polymerising the monomer in the presence of the compound or metal chelate.

IT 46755-84-4 (reaction of, in fluorescent compd. prepn.)

RN 46755-84-4 USPATFULL
CN Borate(1-), hydrotris(1H-pyrazolato- κ .N1)-, (T-4)- (9CI) (CA INDEX NAME)



L14 ANSWER 18 OF 28 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1995:846165 CAPLUS

DOCUMENT NUMBER: 123:305125

TITLE: Synthesis, characterization and reactivity of lanthanide(III) poly(pyrazol-1-yl)borates (Ln = Sm, Eu and Yb); fluorescence studies of [EuL2(THF)2] (L = B(pz)4 HB(pz)3); x-ray crystal structures of [Eu(B(pz)4)2(THF)2] and [Yb(B(pz)4)3]. C2H5OH

AUTHOR(S): Domingos, Angela; Marcalo, Joaquim; Marques, Noemia; Pires De Matos, A.; Galvao, Adelino; Isolani, P. C.; Vicentini, G.; Zinner, K.

CORPORATE SOURCE: Departamento de Quimica, ICEN/INETI, Sacavem, 2686, Port.

SOURCE: Polyhedron (1995), 14(20/21), 3067-76

CODEN: PLVHDE; ISSN: 0277-5387

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The reaction [LnI2(THF)x] (Ln = Sm, Eu, Yb) with 2 equiv of K[B(pz)4] (pz = pyrazolyl) in THF gave [Ln(B(pz)4)2(THF)2] complexes. The mol. structure of [Eu(B(pz)4)2(THF)2] was detd. by single-crystal x-ray diffraction anal. The [Sm(B(pz)4)2(THF)2] and [Yb(B(pz)4)2(THF)2] complexes are fluxional in soln., as indicated by the equivalence of the pyrazolyl rings in the 1H NMR spectra at room temp. A static spectrum could be obtained for the Sm compd. at -68.degree. with a pattern that is in accordance with the geometry found for the Eu complex, in the solid state. [Ln(HB(pz)3)2(THF)2] (Ln = Sm, Eu, Yb) were prepd. by the procedure used to synthesize the [Ln(B(pz)4)2(THF)2] complexes. The THF mols. can be replaced by 1,2-dimethoxyethane yielding [Ln(HB(pz)3)2(DME)] (Ln = Sm, Yb). [Sm(B(pz)4)2(THF)2] and [Yb(B(pz)4)2(THF)2] react readily with alkyl halides, alcs. or alkynes to yield LnIII complexes that disproportionate to the [Ln(B(pz)4)3] complexes. The crystal structure

of [Yb(B(pz)4)3]. EtOH obtained in the reaction of [Yb(B(pz)4)2(THF)2] with EtOH was detd. by x-ray diffraction anal. Fluorescence studies on the Eu compds. are also reported.

IT 14782-58-2, Potassium tetrapyrazolylborate 18583-60-3, Potassium hydrotris(pyrazolyl)borate

RL: RCT (Reactant)

(prepn. of lanthanide(III) poly(pyrazolyl)borates)

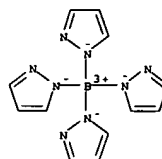
RN 14782-58-2 CAPLUS

CN Borate(1-), tetrakis(1H-pyrazolato-.kappa.N1)-, potassium (9CI) (CA

INDEX

NAME)

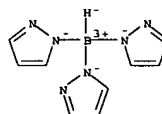
L14 ANSWER 18 OF 28 CAPLUS COPYRIGHT 2002 ACS (Continued)



● K+

RN 18583-60-3 CAPLUS

CN Borate(1-), hydrotris(1H-pyrazolato-.kappa.N1)-, potassium, (T-4)- (9CI) (CA INDEX NAME)



● K+

L14 ANSWER 19 OF 28 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1995:716074 CAPLUS

DOCUMENT NUMBER: 123:286113

TITLE: Recent advances in the chemistry of f-element poly(pyrazolyl)borate complexes

AUTHOR(S): Santos, Isabel; Marques, Naemia

CORPORATE SOURCE: Departamento de Quimica, ICEN-INETI, Port.

SOURCE: New J. Chem. (1995), 19(5-6), 551-71

CODEN: NJCHES; ISSN: 1144-0546

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB This paper presents an overview of the chem. progress involving f-elements and poly(pyrazolyl)borate ligands. This includes compds. of lanthanides(III) and (II) and actinides(IV) and (III). Because of its close similarity, yttrium is also included. The synthetic, chem., structural, and soln. behaviors of these compds. are reviewed with 93 refs.

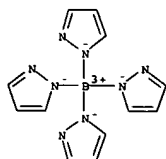
IT 40250-95-1D, Tetrapyrazolyl borate, lanthanide and actinide complexes 46755-84-4D, Hydrotripyrazolyl borate, lanthanide and actinide complexes

RL: PRP (Properties)

(chem. of)

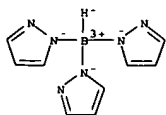
RN 40250-95-1 CAPLUS

CN Borate(1-), tetrakis(1H-pyrazolato-.kappa.N1)- (9CI) (CA INDEX NAME)



RN 46755-84-4 CAPLUS

CN Borate(1-), hydrotris(1H-pyrazolato-.kappa.N1)-, (T-4)- (9CI) (CA INDEX NAME)



L14 ANSWER 20 OF 28 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1995:330153 CAPLUS

DOCUMENT NUMBER: 122:198107

TITLE: Steric control of selectivity for lanthanoids in liquid-liquid extraction with tria- and tetrakis(pyrazol-1-yl)borate-.beta.-diketone mixed-ligand systems

AUTHOR(S): Kokusen, Hisao; Sohrin, Yoshiki; Hasegawa, Hiroshi;

Kihara, Sorin; Matsui, Masakazu

CORPORATE SOURCE: Inst. Chem. Res., Kyoto Univ., Kyoto, 611, Japan

SOURCE: Bull. Chem. Soc. Jpn. (1995), 68(1), 172-7

CODEN: BCSJAS; ISSN: 0009-2673

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Mixed-ligand chelate extn. of trivalent lanthanoid ions (M3+) into benzene

with poly(pyrazol-1-yl)borate (HnB(pz)4-n; n = 0, 1) and .beta.-diketone was studied. The .beta.-diketones used were dibenzoylmethane (dbm) and dipivaloylmethane (dpm). Lanthanoid ions were extd. as [M(HnB(pz)4-n)2(.beta.-diketone)]. The logarithmic extn. const. (log Kex) of the [HB(pz)3]- systems were 5-6 higher than those of the [B(pz)4]- systems.

The highest separability for lanthanoid ions was achieved with the [B(pz)4]-dbm system. These features of log Kex were principally governed by intra- and inter-ligand steric contact.

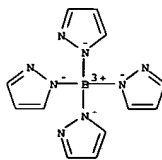
IT 40250-95-1 46755-84-4

RL: ARU (Analytical role, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); ANST (Analytical study); PROC (Process)

(extn. of lanthanoid ions by tria- and tetrakis(pyrazol-1-yl)borate-.beta.-diketone mixed-ligand systems)

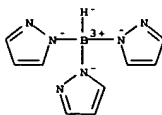
RN 40250-95-1 CAPLUS

CN Borate(1-), tetrakis(1H-pyrazolato-.kappa.N1)- (9CI) (CA INDEX NAME)



RN 46755-84-4 CAPLUS

CN Borate(1-), hydrotris(1H-pyrazolato-.kappa.N1)-, (T-4)- (9CI) (CA INDEX NAME)

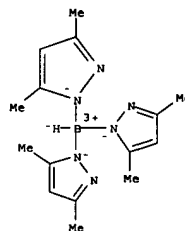


L14 ANSWER 20 OF 28 CAPLUS COPYRIGHT 2002 ACS (Continued)

L14 ANSWER 21 OF 28 CAPLUS COPYRIGHT 2002 ACS

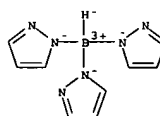
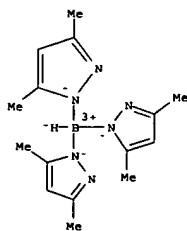
ACCESSION NUMBER: 1994:449074 CAPLUS
 DOCUMENT NUMBER: 121:49074
 TITLE: Synthesis and molecular structures of a redox-related pair of lanthanide complexes
 AUTHOR(S): Maunier, Graham H.; Sella, Andrea; Tocher, Derek A.
 CORPORATE SOURCE: Dep. Chem., UCL, London, WC1H 0AJ, UK
 SOURCE: J. Chem. Soc., Chem. Commun. (1994), (7), 885-6
 CODEN: JCCCAT; ISSN: 0022-4936
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The syntheses and x-ray crystal structures of the isoleptic Yb complexes [Yb(tdmp)2]O3SCP3 and [Yb(tdmp)2] are reported [tdmp = hydrottris(3,5-dimethylpyrazol-1-yl)borate]; the av. metal to ligand distance increases by 0.16 Å. (apprx. 7%) upon redn.
 IT 17567-17-8, Potassium hydrottris(3,5-dimethylpyrazol-1-yl)borate
 RL: RCT (Reactant)
 (reaction of, with ytterbium(III) and (III) compds.)
 RN 17567-17-8 CAPLUS
 CN Borate(1-), tris(3,5-dimethyl-1H-pyrazolato- κ N1)hydro-, potassium, (T-4)- (9CI) (CA INDEX NAME)

● K⁺

L14 ANSWER 22 OF 28 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1994:509072 CAPLUS
 DOCUMENT NUMBER: 121:109072
 TITLE: Cyclooctatetraenyl complexes of early transition metals and lanthanides. V. Synthesis and structure of monocyclooctatetraenyl complex of trivalent titanium
 AUTHOR(S): Kilimann, Ulrike; Noltemeyer, Mathias; Schaefer, Martina; Herbst-Irmer, Regine; Schmidt, Hans-Georg; Edlmann, Frank T.
 CORPORATE SOURCE: Institut fuer Anorganische Chemie der Universitaet Goettingen, Tammannstr. 4, Goettingen, D-37077, Germany
 SOURCE: J. Organomet. Chem. (1994), 469(2), C27-C30
 CODEN: JORCAI; ISSN: 0022-328X
 DOCUMENT TYPE: Journal
 LANGUAGE: German
 OTHER SOURCE(S): CASREACT 121:109072
 AB [(COT)Ti(.mu.-Cl)(THF)]2 (1) reacts with K[HBpz3] or K[HB(3,5-Me2pz)3] to give the new monocyclooctatetraenyl half-sandwich complexes (COT)Ti[HBpz3] (2) and (COT)Ti[HB(3,5-Me2pz)3] (3) resp., as dark green, air-sensitive solids (COT = eta.8-cyclooctatetraenyl(2-)). The mol. structure of 2 has been detd. by an x-ray diffraction study. The monomeric organotitanium(III) complexes (COT)Ti[PhC(NSiMe3)2](THF), (COT)Ti[MeOC6H4C(NSiMe3)2](THF) and (COT)Ti[Ph2P(NSiMe3)2] were prepd. by treatment of 1 with the corresponding heteroallylic ligands.
 IT 17567-17-8 18583-60-3
 RL: RCT (Reactant)
 (reaction of, with cyclooctatetraenyltitanium chloro complex)
 RN 17567-17-8 CAPLUS
 CN Borate(1-), tris(3,5-dimethyl-1H-pyrazolato- κ N1)hydro-, potassium, (T-4)- (9CI) (CA INDEX NAME)

L14 ANSWER 22 OF 28 CAPLUS COPYRIGHT 2002 ACS (Continued)
(CA INDEX NAME)● K⁺● K⁺

RN 18583-60-3 CAPLUS
 CN Borate(1-), hydrottris(1H-pyrazolato- κ N1)-, potassium, (T-4)- (9CI)

L14 ANSWER 23 OF 28 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1994:590859 CAPLUS
 DOCUMENT NUMBER: 121:190859
 TITLE: Fluorescent compounds
 INVENTOR(S): Bell, Colin David; Howse, John Hower C.
 PATENT ASSIGNEE(S): Amersham International PLC, UK
 SOURCE: Eur. Pat. Appl., 33 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 556005	A1	19930818	EP 1993-300892	19930208
EP 556005	B1	19960417		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
EP 688849	A2	19951227	EP 1995-115390	19930208
EP 688849	A3	19960717		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
AT 136925	E	19960515	AT 1993-300892	19930208
CA 2089198	AA	19930815	CA 1993-2089198	19930210
PRIORITY APPLN. INFO.:				
MARPAT 121:190859				
EP 1992-301249 19920214				
EP 1993-300892 19930208				

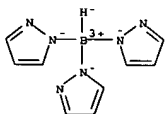
OTHER SOURCE(S):
 AB Comps. are described which are produced by reacting an imido reactant described by the general formula O:Q(R)2N:Z (Q may be the same or different in different parts of the mol. and is selected from P, As, or Sb; R may be the same or different in different parts of the mol. and selected from arom. or heterocyclic rings which may be substituted or unsubstituted, and 1 group R may alternatively be a copolymerizable

group; and Z = OR3 or an oligophosphonyl group) with a chelate of a transition, lanthanide, or actinide metal to produce a product which fluoresces on exposure to UV radiation. Polymer bodies contg. the products are also described which fluoresce on exposure to radiation, as are polymer bodies contg. chelates of transition, lanthanide, or actinide metals which emit light as a result of exposure to internally generated (e.g., from tritium contained in the body) ionizing radiation.

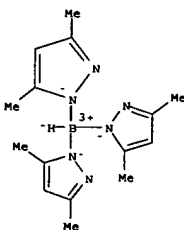
IT 46755-84-4
 RL: RCT (Reactant)
 (reaction of, in fluorescent compd. prepn.)
 RN 46755-84-4 CAPLUS
 CN Borate(1-), hydrotris(1H-pyrazolato-.kappa.N1)-, (T-4)- (9CI) (CA INDEX NAME)

L14 ANSWER 24 OF 28 CAPLUS COPYRIGHT 2002 ACS

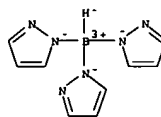
ACCESSION NUMBER: 1991:685120 CAPLUS
 DOCUMENT NUMBER: 119:285120
 TITLE: Polypyrazolylborate derivatives of the lanthanides. The syntheses of oxidation state(II) complexes
 AUTHOR(S): Moss, Michael A. J.; Kresinski, Roman A.; Jones, Christopher J.; Evans, William J.
 CORPORATE SOURCE: Sch. Chem., Univ. Birmingham, Edgbaston/Birmingham, B15 2TT, UK
 SOURCE: Polyhedron (1993), 12(15), 1953-5
 CODEN: PLYHDE; ISSN: 0277-5387
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Air-sensitive bivalent Eu, Sm and Yb complexes were prepd. with the hydrotrispyrazolylborate and hydrotris(3,5-dimethylpyrazolyl)borate ligands and some reactions with CO, propene and (Me2NCS)2 were studied.
 IT 46755-84-4DDP, europium and samarium and ytterbium complexes
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and reactivity of divalent)
 RN 46755-84-4 CAPLUS
 CN Borate(1-), hydrotris(1H-pyrazolato-.kappa.N1)-, (T-4)- (9CI) (CA INDEX NAME)



IT 83534-02-5DDP, europium and samarium and ytterbium complexes
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 83534-02-5 CAPLUS
 CN Borate(1-), tris(3,5-dimethyl-1H-pyrazolato-.kappa.N1)hydro-, (T-4)- (9CI)
 (CA INDEX NAME)

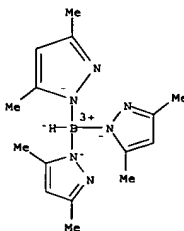


L14 ANSWER 23 OF 28 CAPLUS COPYRIGHT 2002 ACS (Continued)

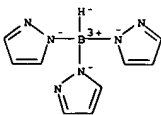


L14 ANSWER 24 OF 28 CAPLUS COPYRIGHT 2002 ACS (Continued)

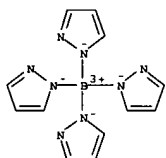
IT 17567-17-8 18583-60-3, Potassium hydrotris(pyrazolyl)borate(1-)
 RL: RCT (Reactant)
 (reaction of, with lanthanide(II) halides)
 RN 17567-17-8 CAPLUS
 CN Borate(1-), tris(3,5-dimethyl-1H-pyrazolato-.kappa.N1)hydro-, potassium, (T-4)- (9CI) (CA INDEX NAME)

● K⁺

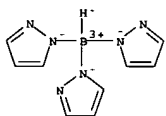
RN 18583-60-3 CAPLUS
 CN Borate(1-), hydrotris(1H-pyrazolato-.kappa.N1)-, potassium, (T-4)- (9CI)
 (CA INDEX NAME)

● K⁺

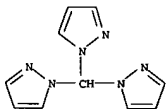
L14 ANSWER 25 OF 28 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1991:220152 CAPLUS
 DOCUMENT NUMBER: 114:220152
 TITLE: Poly(pyrazolyl)borate complexes of selected lanthanide and main group metals
 AUTHOR(S): Knox, Steven Jon
 CORPORATE SOURCE: Univ. South Carolina, Columbia, SC, USA
 SOURCE: (1990) 169 pp. Avail.: Univ. Microfilms Int., Order No. DA9101474
 From: Diss. Abstr. Int. B 1991, 51(8), 3836
 DOCUMENT TYPE: Dissertation
 LANGUAGE: English
 AB Unavailable
 IT 40250-95-1 CAPLUS
 complexes 46755-84-4DP, lanthanide and main group metal complexes
 RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)
 RN 40250-95-1 CAPLUS
 CN Borate(1-), tetrakis(1H-pyrazolato-.kappa.N1)- (9CI) (CA INDEX NAME)



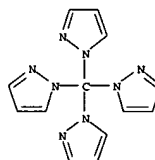
RN 46755-84-4 CAPLUS
 CN Borate(1-), hydrotris(1H-pyrazolato-.kappa.N1)-, (T-4)- (9CI) (CA INDEX NAME)



L14 ANSWER 26 OF 28 CAPLUS COPYRIGHT 2002 ACS (Continued)

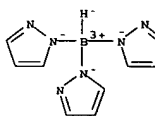


L14 ANSWER 26 OF 28 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1990:458164 CAPLUS
 DOCUMENT NUMBER: 113:58164
 TITLE: A conformational study of bis-, tri- and tetrakis(pyrazolyl)methane. Crystallography, lanthanide shift reagents, dipole moments and theoretical calculations
 AUTHOR(S): Claramunt, Rosa Maria; Elguero, Jose; Fabre, Maria Jose; Foces-Foces, Concepcion; Hernandez Cano, Felix; Hernandez Fuentes, Irmira; Jaime, Carlos; Lopez, Concepcion
 CORPORATE SOURCE: Fac. Cienc., UNED, Madrid, 28040, Spain
 SOURCE: Tetrahedron (1989), 45(24), 7805-16
 CODEN: TETRA8; ISSN: 0040-4020
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Theor. calcns. (M02 and MNDO) have been carried out on several conformations of di-, tri- and tetrapyrazolylmethane. The potential surface thus obtained has been compared with exptl. results both in soln. (lanthanide shift reagents, dipole moments) and in the solid state (crystallog.). The structure of tetrapyrazolylmethane was detd. by x-ray diffraction. The mol. presents an approx. S4(4) axis such as N-12, N-22, N-43 and N-42 form a distorted tetrahedron. The calcd. conformations of min. energy are consistent with dielec. measurements. The structure of 3 in the solid state lies 5.0 kcal.mol-1 above the min. as a result of the crystal field. To explain the LSR results, a coordination with two pyrazole nuclei has to be assumed. The presence of a metal (LSR, organometallic complexes) strongly modifies the conformation: in these conditions, bidentated and tridentated structures are obsd.
 IT 28791-96-0 80510-03-8
 RL: PRP (Properties) (conformational anal. of)
 RN 28791-96-0 CAPLUS
 CN 1H-Pyrazole, 1,1',1'',1'''-methanetetrayltetrakis- (9CI) (CA INDEX NAME)



RN 80510-03-8 CAPLUS
 CN 1H-Pyrazole, 1,1',1'',1'''-methyldynetris- (9CI) (CA INDEX NAME)

L14 ANSWER 27 OF 28 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1989:469702 CAPLUS
 DOCUMENT NUMBER: 111:69702
 TITLE: Heteroleptic polypyrazolylborate complexes of the lanthanide ions. The synthesis of carboxylate complexes and the molecular structure of [Yb(HB(C3N2H3)3)2(O2CPh)]
 AUTHOR(S): Moss, Michael A. J.; Jones, Christopher J.
 CORPORATE SOURCE: Dep. Chem., Univ. Birmingham, Birmingham, B15 2TT, UK
 SOURCE: Polyhedron (1989), 8(4), 555-8
 CODEN: PLYHDE; ISSN: 0277-5387
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The heteroleptic lanthanide ion complexes [LnL2X] (L = HB(pz)3 (pz = pyrazolyl) Ln = Y, Sm, Eu, Yb, Lu and X = OBz; Ln = Y, Yb, Lu and X = OAc) were prepd. and characterized. They are monomeric and a single crystal x-ray diffraction study of [YbL2(O2CPh)] [triclinic, space group P.hvln.1, a 9.148(1), b 15.796(8), c 20.089(10) .ANG., .alpha. 81.57(5), .beta. 88.65(2), .gamma. 88.15(3) .degree., Z = 4, dc = 1.67 g cm-3, R = 0.0504, Rw = 0.0519] shows that the mol. has a distorted square antiprismatic (SAP) coordination geometry which lies on the geometric pathway from SAP to dodecahedral. The av. Yb-O distance is 2.33(2) .ANG. and the av. Yb-N distance is 2.43(4) .ANG.. [LnL2(X1)LnL2] (Ln = Y, Yb, Lu and X1 = O2CCO2) were also prepd.
 IT 46755-84-4DP, rare earth metal complexes with benzoate (prepn. of)
 RN 46755-84-4 CAPLUS
 CN Borate(1-), hydrotris(1H-pyrazolato-.kappa.N1)-, (T-4)- (9CI) (CA INDEX NAME)



L14 ANSWER 28 OF 28 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1989:545717 CAPLUS

DOCUMENT NUMBER: 111:145717

TITLE: Lanthanide coordination chemistry:
spectroscopic properties of terbium and europium
poly(pyrazol-1-yl)- and poly(imidazol-1-yl)borate
complexes

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AB Complexes formed between $H_4-xBRx-$ ($R = 1$ -pyrazolyl (pz), 1-imidazolyl (IM); $n = 2, 3, 4$) and Tb^{3+} or Eu^{3+} were examd. by IR, UV absorption, and emission spectroscopy. HBR_3- and BR_4- yielded isostructural compds. with both lanthanides, but having a different mol. geometry than the H_2BR_2- complexes. Electronic spectra indicate that the $H_4-xB(pz)_x-$ complexes emit from a ligand-to-metal (LMCT) charge transfer state. The free ligands are UV transparent however, suggesting that the sensitizing chromophore responsible for emission is created only upon complex formation. The $H_4-xB(IM)_x-$ compds. exhibit a more complicated excited state profile, with emission apparently originating from both

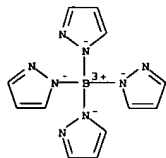
LMCT and intraligand states.

IT 40250-95-1DP, Tetra(1-pyrazolyl)borate, europium and terbium
complexes 46755-84-4DP, Hydrotris(1-pyrazolyl)borate, europium
and terbium complexes

RL: PRP (Properties); PREP (Preparation)
(formation and spectra of)

RN 40250-95-1 CAPLUS

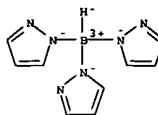
CN Borate(1-), tetrakis(1H-pyrazolato-.kappa.N1)- (9CI) (CA INDEX NAME)

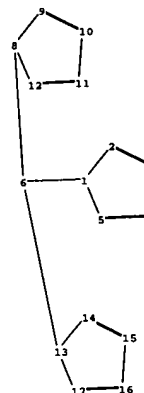
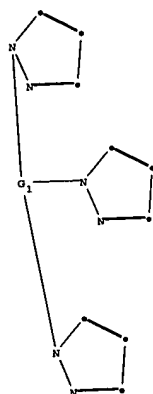


RN 46755-84-4 CAPLUS

CN Borate(1-), hydrotris(1H-pyrazolato-.kappa.N1)-, (T-4)- (9CI) (CA INDEX
NAME)

L14 ANSWER 28 OF 28 CAPLUS COPYRIGHT 2002 ACS (Continued)





chain nodes :

6

ring nodes :

1 2 3 4 5 8 9 10 11 12 13 14 15 16 17

chain bonds :

1-6 6-8 6-13

ring bonds :

1-2 1-5 2-3 3-4 4-5 8-9 8-12 9-10 10-11 11-12 13-14 13-17 14-15 15-16 16-17

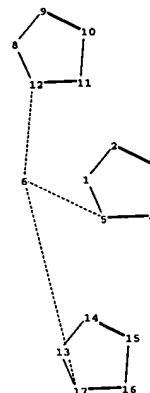
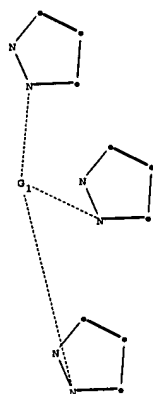
exact/norm bonds :

1-2 1-5 1-6 2-3 3-4 4-5 6-8 6-13 8-9 8-12 9-10 10-11 11-12 13-14 13-17 14-15
15-16 16-17

G1:C,B

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom
13:Atom 14:Atom 15:Atom 16:Atom 17:Atom



chain nodes :

6

ring nodes :

1 2 3 4 5 8 9 10 11 12 13 14 15 16 17

chain bonds :

5-6 6-17 6-12

ring bonds :

1-2 1-5 2-3 3-4 4-5 8-9 8-12 9-10 10-11 11-12 13-14 13-17 14-15 15-16 16-17

exact/norm bonds :

1-2 1-5 2-3 3-4 4-5 5-6 6-17 6-12 8-9 8-12 9-10 10-11 11-12 13-14 13-17
14-15 15-16 16-17

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